CS 391L: Machine Learning: Computational Learning Theory

Raymond J. Mooney

University of Texas at Austin

Learning Theory

- Theorems that characterize classes of learning problems or specific algorithms in terms of computational complexity or ***sample complexity***, i.e. the number of training examples necessary or sufficient to learn hypotheses of a given accuracy.
- Complexity of a learning problem depends on:
  - Size or expressiveness of the hypothesis space.
  - Accuracy to which target concept must be approximated.
  - Probability with which the learner must produce a successful hypothesis.
  - Manner in which training examples are presented, e.g. randomly or by query to an oracle.

Types of Results

- **Learning in the limit**: Is the learner guaranteed to converge to the correct hypothesis in the limit as the number of training examples increases indefinitely?
- **Sample Complexity**: How many training examples are needed for a learner to construct (with high probability) a highly accurate concept?
- **Computational Complexity**: How much computational resources (time and space) are needed for a learner to construct (with high probability) a highly accurate concept?
  - High sample complexity implies high computational complexity, since learner at least needs to read the input data.
- **Mistake Bound**: Learning incrementally, how many training examples will the learner misclassify before constructing a highly accurate concept.

Learning in the Limit

- Given a continuous stream of examples where the learner predicts whether each one is a member of the concept or not and is then is told the correct answer, does the learner eventually converge to a correct concept and never make a mistake again.
- No limit on the number of examples required or computational demands, but must eventually learn the concept exactly, although do not need to explicitly recognize this convergence point.
- By simple enumeration, concepts from any known finite hypothesis space are learnable in the limit, although typically requires an exponential (or doubly exponential) number of examples and time.
- Class of total recursive (Turing computable) functions is not learnable in the limit.

Unlearnable Problem

- Identify the function underlying an ordered sequence of natural numbers ($t: \mathcal{N} \rightarrow \mathcal{N}$), guessing the next number in the sequence and then being told the correct value.
- For any given learning algorithm L, there exists a function $t(n)$ that it cannot learn in the limit.

Given the learning algorithm L as a Turing machine:

$$D \rightarrow \boxed{L} \rightarrow h(n)$$

Construct a function it cannot learn:

$$t(n) \left\{ \begin{array}{c} \langle t(0), t(1), \ldots t(n-1) \rangle \\ \downarrow \\ \boxed{L} \\ \downarrow \\ h(n) + 1 \end{array} \right.$$

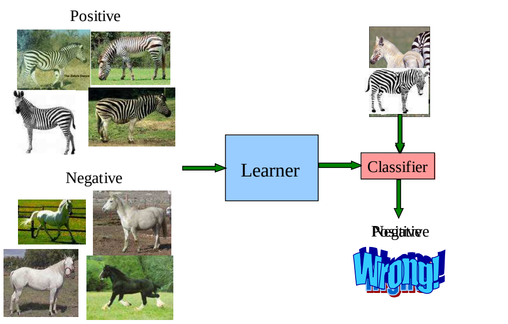
Example Trace

Oracle:	1	3	6	11	…..
Learner:	0	2	5	10	
h:	natural	pos int	odd int	$h(n)=h(n-1)+n+1$	

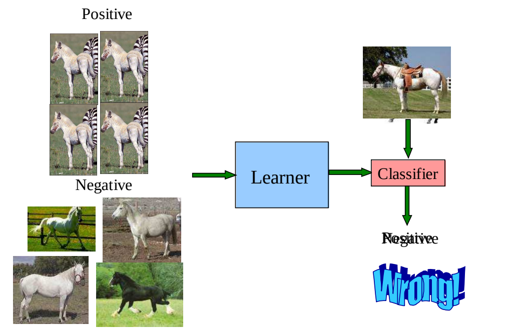
Learning in the Limit vs. PAC Model

- Learning in the limit model is too strong.
  - Requires learning correct exact concept
- Learning in the limit model is too weak
  - Allows unlimited data and computational resources.
- PAC Model
  - Only requires learning a ***Probably Approximately Correct*** Concept: Learn a decent approximation most of the time.
  - Requires polynomial sample complexity and computational complexity.

Cannot Learn Exact Concepts from Limited Data, Only Approximations



Cannot Learn Even Approximate Concepts from Pathological Training Sets



PAC Learning

- The only reasonable expectation of a learner is that with ***high probability*** it learns a ***close approximation*** to the target concept.
- In the PAC model, we specify two small parameters, ε and δ, and require that with probability at least $(1 - \delta)$ a system learn a concept with error at most ε.

Formal Definition of PAC-Learnable

- Consider a concept class C defined over an instance space X containing instances of length n, and a learner, L, using a hypothesis space, H. C is said to be ***PAC-learnable*** by L using H iff for all $c \in C$, distributions D over X, $0<\varepsilon<0.5$, $0<\delta<0.5$; learner L by sampling random examples from distribution D, will with probability at least $1-\delta$ output a hypothesis $h \in H$ such that $\text{error}_D(h) \leq \varepsilon$, in time polynomial in $1/\varepsilon$, $1/\delta$, n and size(c).
- Example:
  - *X:* instances described by *n* binary features
  - *C:* conjunctive descriptions over these features
  - *H*: conjunctive descriptions over these features
  - *L*: most-specific conjunctive generalization algorithm (Find-S)
  - *size(c)*: the number of literals in *c* (i.e. length of the conjunction).

Issues of PAC Learnability

- The computational limitation also imposes a polynomial constraint on the training set size, since a learner can process at most polynomial data in polynomial time.
- How to prove PAC learnability:
  - First prove sample complexity of learning C using H is polynomial.
  - Second prove that the learner can train on a polynomial-sized data set in polynomial time.
- To be PAC-learnable, there must be a hypothesis in H with arbitrarily small error for every concept in C, generally $C \subseteq H$.

Consistent Learners

- A learner L using a hypothesis H and training data D is said to be a consistent learner if it always outputs a hypothesis with zero error on D whenever H contains such a hypothesis.
- By definition, a consistent learner must produce a hypothesis in the version space for H given D.
- Therefore, to bound the number of examples needed by a consistent learner, we just need to bound the number of examples needed to ensure that the version-space contains no hypotheses with unacceptably high error.

ε-Exhausted Version Space

- The version space, $VS_{H,D}$, is said to be ***ε-exhausted*** iff every hypothesis in it has true error less than or equal to ε.
- In other words, there are enough training examples to guarantee than any consistent hypothesis has error at most ε.
- One can never be sure that the version-space is ε-exhausted, but one can bound the probability that it is not.
- **Theorem 7.1** (Haussler, 1988): If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples for some target concept c, then for any $0 \leq \varepsilon \leq 1$, the probability that the version space $VS_{H,D}$ is ***not*** ε-exhausted is less than or equal to:

$$|H|e^{-\varepsilon m}$$

13

Proof

- Let $H_{\text{bad}}=\{h_1,\ldots h_k\}$ be the subset of H with error > ε. The VS is not ε-exhausted if any of these are consistent with all m examples.
- A single $h_i \in H_{\text{bad}}$ is consistent with ***one*** example with probability:

$$P(\text{consist}(h_i, e_j)) \leq (1-\varepsilon)$$

- A single $h_i \in H_{\text{bad}}$ is consistent with ***all*** m independent random examples with probability:

$$P(\text{consist}(h_i, D)) \leq (1-\varepsilon)^m$$

- The probability that ***any*** $h_i \in H_{\text{bad}}$ is consistent with all m examples is:

$$P(\text{consist}(H_{bad}, D)) = P(\text{consist}(h_1, D) \vee \cdots \vee \text{consist}(h_k, D))$$

14

Proof (cont.)

- Since the probability of a disjunction of events is ***at most*** the sum of the probabilities of the individual events:

$$P(\text{consist}(H_{bad}, D)) \leq |H_{bad}|(1-\varepsilon)^m$$

- Since: $|H_{\text{bad}}| \leq |H|$ and $(1-\varepsilon)^m \leq e^{-\varepsilon m}$, $0 \leq \varepsilon \leq 1$, $m \geq 0$

$$P(\text{consist}(H_{bad}, D)) \leq |H|e^{-\varepsilon m}$$

Q.E.D

15

Sample Complexity Analysis

- Let δ be an upper bound on the probability of ***not*** exhausting the version space. So:

$$P(\text{consist}(H_{bad}, D)) \leq |H|e^{-\varepsilon m} \leq \delta$$

$$e^{-\varepsilon m} \leq \frac{\delta}{|H|}$$

$$-\varepsilon m \leq \ln(\frac{\delta}{|H|})$$

$$m \geq \left(-\ln \frac{\delta}{|H|}\right) / \varepsilon \quad \text{(flip inequality)}$$

$$m \geq \left(\ln \frac{|H|}{\delta}\right) / \varepsilon$$

$$m \geq \left(\ln \frac{1}{\delta} + \ln|H|\right) / \varepsilon$$

16

Sample Complexity Result

- Therefore, any consistent learner, given at least:

$$\left(\ln \frac{1}{\delta} + \ln|H|\right) / \varepsilon$$

examples will produce a result that is PAC.
- Just need to determine the size of a hypothesis space to instantiate this result for learning specific classes of concepts.
- This gives a ***sufficient*** number of examples for PAC learning, but ***not*** a ***necessary*** number. Several approximations like that used to bound the probability of a disjunction make this a gross over-estimate in practice.

17

Sample Complexity of Conjunction Learning

- Consider conjunctions over n boolean features. There are 3^n of these since each feature can appear positively, appear negatively, or not appear in a given conjunction. Therefore $|H| = 3^n$, so a sufficient number of examples to learn a PAC concept is:

$$\left(\ln \frac{1}{\delta} + \ln 3^n\right) / \varepsilon = \left(\ln \frac{1}{\delta} + n \ln 3\right) / \varepsilon$$

- Concrete examples:
  - δ=ε=0.05, n=10 gives 280 examples
  - δ=0.01, ε=0.05, n=10 gives 312 examples
  - δ=ε=0.01, n=10 gives 1,560 examples
  - δ=ε=0.01, n=50 gives 5,954 examples
- Result holds for any consistent learner, including FindS.

18

Sample Complexity of Learning Arbitrary Boolean Functions

- Consider any boolean function over n boolean features such as the hypothesis space of DNF or decision trees. There are 2^{2^n} of these, so a sufficient number of examples to learn a PAC concept is:

$$\left(\ln\frac{1}{\delta}+\ln 2^{2^n}\right)/\varepsilon=\left(\ln\frac{1}{\delta}+2^n\ln 2\right)/\varepsilon$$

- Concrete examples:
  - δ=ε=0.05, n=10 gives 14,256 examples
  - δ=ε=0.05, n=20 gives 14,536,410 examples
  - δ=ε=0.05, n=50 gives 1.561×10^{16} examples

19

Other Concept Classes

- k-term DNF: Disjunctions of at most k unbounded conjunctive terms: $T_1 \vee T_2 \vee \cdots \vee T_k$
  - ln(|H|)=O(kn)
- k-DNF: Disjunctions of any number of terms each limited to at most k literals: $((L_1 \wedge L_2 \wedge \cdots \wedge L_k) \vee (M_1 \wedge M_2 \wedge \cdots \wedge M_k) \vee \cdots$
  - ln(|H|)=O(n^k)
- k-clause CNF: Conjunctions of at most k unbounded disjunctive clauses: $C_1 \wedge C_2 \wedge \cdots \wedge C_k$
  - ln(|H|)=O(kn)
- k-CNF: Conjunctions of any number of clauses each limited to at most k literals: $((L_1 \vee L_2 \vee \cdots \vee L_k) \wedge (M_1 \vee M_2 \vee \cdots \vee M_k) \wedge \cdots$
  - ln(|H|)=O(n^k)

Therefore, all of these classes have polynomial sample complexity given a fixed value of k.

20

Basic Combinatorics Counting

	dups allowed	dups not allowed
order relevant	samples	permutations
order irrelevant	selections	combinations

Pick 2 from {a,b}

samples	permutations	selections	combinations
aa	ab	aa	ab
ab	ba	ab	
ba		bb	
bb			

$$\text{k-samples}: n^k \qquad \text{k-selections}: \binom{n+k-1}{k}=\frac{(n+k-1)!}{k!(n-1)!}$$

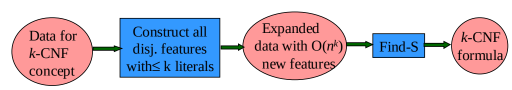
$$\text{k-permutations}: \frac{n!}{(n-k)!} \qquad \text{k-combinations}: \binom{n}{k}=\frac{n!}{k!(n-k)!}$$

All O(n^k)

21

Computational Complexity of Learning

- However, determining whether or not there exists a k-term DNF or k-clause CNF formula consistent with a given training set is NP-hard. Therefore, these classes are not PAC-learnable due to computational complexity.
- There are polynomial time algorithms for learning k-CNF and k-DNF. Construct all possible disjunctive clauses (conjunctive terms) of at most k literals (there are O(n^k) of these), add each as a new constructed feature, and then use FIND-S (FIND-G) to find a purely conjunctive (disjunctive) concept in terms of these complex features.

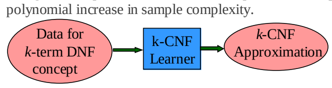


Sample complexity of learning k-DNF and k-CNF are O(n^k)
Training on O(n^k) examples with O(n^k) features takes O(n^{2k}) time

22

Enlarging the Hypothesis Space to Make Training Computation Tractable

- However, the language k-CNF is a superset of the language k-term-DNF since any k-term-DNF formula can be rewritten as a k-CNF formula by distributing AND over OR.
- Therefore, C = k-term DNF can be learned using H = k-CNF as the hypothesis space, but it is intractable to learn the concept in the form of a k-term DNF formula (also the k-CNF algorithm might learn a close approximation in k-CNF that is not actually expressible in k-term DNF).
  - Can gain an exponential decrease in computational complexity with only a polynomial increase in sample complexity.



- Dual result holds for learning k-clause CNF using k-DNF as the hypothesis space.

23

Probabilistic Algorithms

- Since PAC learnability only requires an approximate answer with ***high probability***, a probabilistic algorithm that only halts and returns a consistent hypothesis in polynomial time with a high-probability is sufficient.
- However, it is generally assumed that NP complete problems cannot be solved even with high probability by a probabilistic polynomial-time algorithm, i.e. RP ≠ NP.
- Therefore, given this assumption, classes like k-term DNF and k-clause CNF are not PAC learnable in that form.

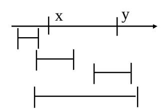
24

Infinite Hypothesis Spaces

- The preceding analysis was restricted to finite hypothesis spaces.
- Some infinite hypothesis spaces (such as those including real-valued thresholds or parameters) are more expressive than others.
  – Compare a rule allowing one threshold on a continuous feature (length<3cm) vs one allowing two thresholds (1cm<length<3cm).
- Need some measure of the expressiveness of infinite hypothesis spaces.
- The ***Vapnik-Chervonenkis*** **(*VC*)** ***dimension*** provides just such a measure, denoted VC(H).
- Analagous to ln|H|, there are bounds for sample complexity using VC(H).

Shattering Instances

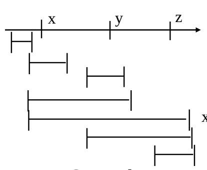
- A hypothesis space is said to shatter a set of instances iff for every partition of the instances into positive and negative, there is a hypothesis that produces that partition.
- For example, consider 2 instances described using a single real-valued feature being shattered by intervals.



+	–
	x,y
x	y
y	x
x,y	

Shattering Instances (cont)

- But 3 instances cannot be shattered by a single interval.



+	–
	x,y,z
x	y,z
y	x,z
x,y	z
x,y,z	
y,z	x
z	x,y
x,z	y

Cannot do

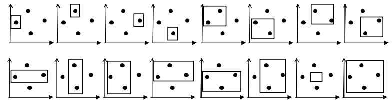
- Since there are 2^m partitions of m instances, in order for H to shatter instances: $|H| \geq 2^m$.

VC Dimension

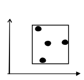
- An unbiased hypothesis space shatters the entire instance space.
- The larger the subset of X that can be shattered, the more expressive the hypothesis space is, i.e. the less biased.
- The Vapnik-Chervonenkis dimension, VC(H). of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite subsets of X can be shattered then VC(H) = ∞
- If there exists at least one subset of X of size d that can be shattered then VC(H) ≥ d. If no subset of size d can be shattered, then VC(H) < d.
- For a single intervals on the real line, all sets of 2 instances can be shattered, but no set of 3 instances can, so VC(H) = 2.
- Since $|H| \geq 2^m$, to shatter m instances, VC(H) ≤ $\log_2|H|$

VC Dimension Example

- Consider axis-parallel rectangles in the real-plane, i.e. conjunctions of intervals on two real-valued features. Some 4 instances can be shattered.

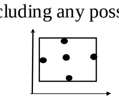


Some 4 instances cannot be shattered:



VC Dimension Example (cont)

- No five instances can be shattered since there can be at most 4 distinct extreme points (min and max on each of the 2 dimensions) and these 4 cannot be included without including any possible 5[th] point.



- Therefore VC(H) = 4
- Generalizes to axis-parallel hyper-rectangles (conjunctions of intervals in n dimensions): VC(H)=2n.

Upper Bound on Sample Complexity with VC

- Using VC dimension as a measure of expressiveness, the following number of examples have been shown to be sufficient for PAC Learning (Blumer *et al.*, 1989).

$$\frac{1}{\varepsilon}\left(4\log_2\left(\frac{2}{\delta}\right)+8VC(H)\log_2\left(\frac{13}{\varepsilon}\right)\right)$$

- Compared to the previous result using ln|*H*|, this bound has some extra constants and an extra $\log_2(1/\varepsilon)$ factor. Since $VC(H) \leq \log_2|H|$, this can provide a tighter upper bound on the number of examples needed for PAC learning.

Conjunctive Learning with Continuous Features

- Consider learning axis-parallel hyper-rectangles, conjunctions on intervals on *n* continuous features.
  - $1.2 \leq \text{length} \leq 10.5 \wedge 2.4 \leq \text{weight} \leq 5.7$
- Since VC(*H*)=2*n* sample complexity is

$$\frac{1}{\varepsilon}\left(4\log_2\left(\frac{2}{\delta}\right)+16n\log_2\left(\frac{13}{\varepsilon}\right)\right)$$

- Since the most-specific conjunctive algorithm can easily find the tightest interval along each dimension that covers all of the positive instances ($f_{min} \leq f \leq f_{max}$) and runs in linear time, O(|*D*|*n*), axis-parallel hyper-rectangles are PAC learnable.

Sample Complexity Lower Bound with VC

- There is also a general lower bound on the minimum number of examples necessary for PAC learning (Ehrenfeucht, *et al.*, 1989):

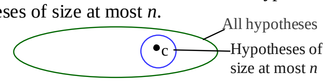
  Consider any concept class *C* such that VC(*H*)≥2 any learner *L* and any 0<ε<1/8, 0<δ<1/100. Then there exists a distribution *D* and target concept in *C* such that if *L* observes fewer than:

$$\max\left(\frac{1}{\varepsilon}\log_2\left(\frac{1}{\delta}\right),\frac{VC(C)-1}{32\varepsilon}\right)$$

  examples, then with probability at least δ, *L* outputs a hypothesis having error greater than ε.
- Ignoring constant factors, this lower bound is the same as the upper bound except for the extra $\log_2(1/\varepsilon)$ factor in the upper bound.

Analyzing a Preference Bias

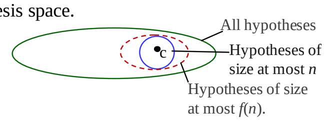
- Unclear how to apply previous results to an algorithm with a preference bias such as simplest decisions tree or simplest DNF.
- If the size of the correct concept is *n*, and the algorithm is guaranteed to return the minimum sized hypothesis consistent with the training data, then the algorithm will always return a hypothesis of size at most *n*, and the effective hypothesis space is all hypotheses of size at most *n*.



- Calculate |*H*| or VC(*H*) of hypotheses of size at most *n* to determine sample complexity.

Computational Complexity and Preference Bias

- However, finding a minimum size hypothesis for most languages is computationally intractable.
- If one has an approximation algorithm that can bound the size of the constructed hypothesis to some polynomial function, *f*(*n*), of the minimum size *n*, then can use this to define the effective hypothesis space.



- However, no worst case approximation bounds are known for practical learning algorithms (e.g. ID3).

"Occam's Razor" Result (Blumer *et al.*, 1987)

- Assume that a concept can be represented using at most *n* bits in some representation language.
- Given a training set, assume the learner returns the consistent hypothesis representable with the least number of bits in this language.
- Therefore the effective hypothesis space is all concepts representable with at most *n* bits.
- Since *n* bits can code for at most 2^n hypotheses, $|H|=2^n$, so sample complexity if bounded by:

$$\left(\ln\frac{1}{\delta}+\ln 2^n\right)/\varepsilon=\left(\ln\frac{1}{\delta}+n\ln 2\right)/\varepsilon$$

- This result can be extended to approximation algorithms that can bound the size of the constructed hypothesis to at most n^k for some fixed constant *k* (just replace *n* with n^k)

Interpretation of "Occam's Razor" Result

- Since the encoding is unconstrained it fails to provide any meaningful definition of "simplicity."
- Hypothesis space could be any sufficiently small space, such as "the 2^n most complex boolean functions, where the complexity of a function is the size of its smallest DNF representation"
- Assumes that the correct concept (or a close approximation) is actually in the hypothesis space, so assumes *a priori* that the concept is simple.
- Does not provide a theoretical justification of Occam's Razor as it is normally interpreted.

37

COLT Conclusions

- The PAC framework provides a theoretical framework for analyzing the effectiveness of learning algorithms.
- The sample complexity for any consistent learner using some hypothesis space, H, can be determined from a measure of its expressiveness $|H|$ or VC(H), quantifying bias and relating it to generalization.
- If sample complexity is tractable, then the computational complexity of finding a consistent hypothesis in H governs its PAC learnability.
- Constant factors are more important in sample complexity than in computational complexity, since our ability to gather data is generally not growing exponentially.
- Experimental results suggest that theoretical sample complexity bounds over-estimate the number of training instances needed in practice since they are worst-case upper bounds.

38

COLT Conclusions (cont)

- Additional results produced for analyzing:
  - Learning with queries
  - Learning with noisy data
  - Average case sample complexity given assumptions about the data distribution.
  - Learning finite automata
  - Learning neural networks
- Analyzing practical algorithms that use a preference bias is difficult.
- Some effective practical algorithms motivated by theoretical results:
  - Boosting
  - Support Vector Machines (SVM)

39